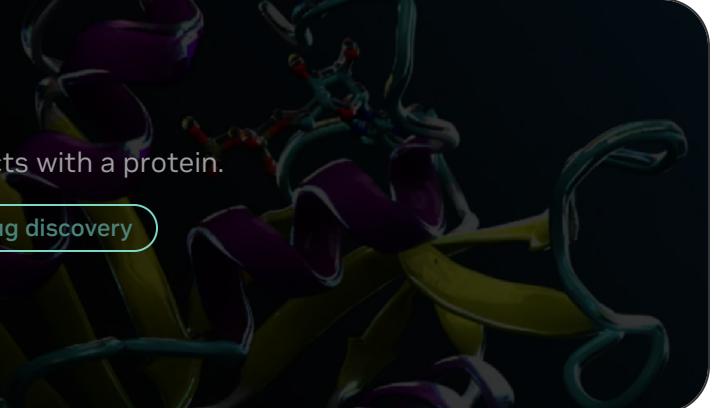


mit
diffdock [Run Anywhere](#)

Predicts the 3D structure of how a molecule interacts with a protein.

bionemo chemistry docking nim drug discovery

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Output Preview Ascii

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Molecule * ⓘ

Ensitrelvir_analog_3d.sdf

File Types: .sdf | .mol2 [Upload New File](#)

```
{"title":"{\"type\":\"urn:inference-service:problem-details:internal-server-error\",\"title\":\"Internal Server Error\",\"status\":500,\"detail\":\"Inference error\"}"]}
```

Target Protein * ⓘ

mpro_chain_OpenFold_proc...

File Types: .pdb [Upload New File](#)

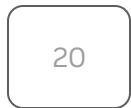
Generated Poses ⓘ

Diffusion Steps ⓘ

1 11 21 31 40
1 3 5 7 9 11 13 15 17 19 20

**Diffusion Time Divisions** ⓘ

3 5 7 9 11 13 15 17 19 20

**Reset****Run**

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